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Physics-Informed Artificial Intelligence for Autonomous Scientific Discovery an Adaptive Framework for Data-Efficient Physical System Modeling

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Abstract

The integration of artificial intelligence with physical knowledge has become an important area of scientific machine learning, particularly for modeling physical systems with limited or noisy data. Physics-informed neural networks (PINNs) incorporate governing physical laws into neural-network training. However, conventional PINNs often face challenges such as optimization difficulties, high computational costs, sensitivity to sampling strategies, and limited generalization. This study proposes an adaptive physics-informed artificial intelligence framework that combines deep neural prediction, governing physical equations, residual-based adaptive sampling, automated error assessment, and iterative model refinement. The framework is evaluated using the one-dimensional transient heat equation under different data availability and noise levels. Three models are compared: a conventional data-driven neural network, a standard PINN, and the proposed adaptive PINN. The results show that the proposed model performs significantly better in sparse-data conditions. With only 1% of the available data, it achieves a relative prediction error of 0.00142 compared with 0.185 for the conventional neural network, representing an improvement of more than two orders of magnitude. It also reduces computational collocation overhead by approximately 4.2 times compared with uniform dense sampling. These findings demonstrate the potential of adaptive physics-informed AI for accurate, data-efficient, and computationally efficient modeling of physical systems.

***Keywords**: Physics-informed artificial intelligence; Physics-informed neural networks; Scientific machine learning; Autonomous scientific discovery; Adaptive sampling*

INTRODUCTION

Artificial intelligence has revolutionized scientific computing by enabling high-capacity neural networks to approximate complex, non-linear spatiotemporal mappings. However, purely data-driven machine learning models suffer from severe vulnerabilities: they require vast labeled datasets, struggle to generalize beyond training distributions, and often generate predictions that violate fundamental conservation laws of physics (e.g., energy, mass, or momentum conservation).

Scientific Machine Learning (SciML) bridges this gap by embedding formal domain knowledge directly into learning algorithms. Physics-Informed Neural Networks (PINNs), popularized by Raissi et al. (2019), leverage automatic differentiation to evaluate partial differential equation (PDE) residuals directly within the loss function. This allows networks to respect governing laws without requiring spatial or temporal discretization meshes. PINNs have shown remarkable promise across heat transfer, fluid dynamics, solid mechanics, geophysics, and inverse problem estimation.

Concurrently, autonomous AI systems are transforming the research process itself. Recent automated AI scientists manage scientific pipelines end-to-end—generating research hypotheses, executing numerical code, analyzing data, generating visualizations, and writing manuscripts. Combining physics-informed constraints with autonomous experimentation loops creates an opportunity for closed-loop, data-efficient scientific discovery.

Problem Statement

Despite their demonstrated capabilities, standard Physics-Informed Neural Network (PINN) formulations exhibit critical limitations that hinder their practical reliability. Fixed, uniform collocation grids frequently under-sample critical regions (e.g., sharp gradients, boundary layers, transient shocks) while over-sampling homogeneous regions, incurring unnecessary computational expense and degrading accuracy in high-error zones. Purely data-driven models fail under extremely sparse observation conditions, while PINNs with unweighted or poorly balanced loss terms are prone to converging on local minima caused by imbalances among the data, PDE residual, and boundary condition losses. Compounding these issues, standard PINN workflows depend on manual, trial-and-error tuning to refine sampling strategies, adjust loss weights, and set training schedules — a process that is time-consuming, non-reproducible, and does not scale to complex or evolving physical systems (Hossen et al., 2026).

Research Gap

Existing paradigms remain bifurcated along two disconnected tracks: standard PINN workflows follow a static, non-adaptive pipeline (Physics Equations → Neural Network → Prediction) with no mechanism for self-correction once training begins, while autonomous AI scientist frameworks (Literature Review → Hypothesis Generation → Code Execution → Manuscript Generation) are capable of autonomous reasoning and iteration but lack any integration of governing physical constraints or PDE-based residual feedback. Neither paradigm alone resolves the limitations above — standard PINNs cannot adapt their own sampling or training strategy, while autonomous AI scientist frameworks are not grounded in physical law. The framework proposed in this study bridges these two fields by introducing a closed-loop, self-refining architecture — Physical System → Physics-Informed Model → Prediction → Residual Analysis → Adaptive Resampling → Model Refinement → Scientific Insight — that embeds autonomous, residual-driven decision-making directly into the physics-constrained training loop, enabling the model to iteratively identify its own regions of highest error, reallocate collocation resources accordingly, and refine itself without manual intervention.

Research Objectives

The general objective of this study is to develop, implement, and experimentally validate an adaptive physics-informed artificial intelligence framework for data-efficient modeling and autonomous physical-system exploration. To achieve this, the study pursues several specific objectives: to design a unified deep learning architecture capable of evaluating spatial and temporal automatic derivatives; to implement a Residual-Based Adaptive Refinement (RAR) algorithm that dynamically concentrates collocation points in regions of maximum physical inconsistency; to systematically benchmark predictive accuracy (MAE, RMSE, relative) across data fractions ranging from 1% to 100%; to quantify model robustness under Gaussian observational noise levels ranging from 0% to 10%; to evaluate out-of-distribution generalization under modified thermal diffusivity and unseen initial boundary functions; and to establish a formal mathematical and computational protocol for autonomous lab-in-the-loop scientific discovery.

Research Questions & Hypotheses

This study addresses six core research questions (RQ1–RQ6):

RQ1: Can adaptive physics-informed learning improve prediction accuracy and data efficiency while maintaining exact physical consistency?
RQ2: How does a PINN compare to a conventional data-driven neural network under severe data scarcity?
RQ3: Does residual-driven adaptive sampling outperform uniform fixed-grid sampling?
RQ4: How robust are physics-informed models against high levels of observational noise?
RQ5: Does the adaptive framework generalize accurately to unseen physical parameters?
RQ6: Can physical residual analysis serve as a valid objective driver for autonomous scientific exploration?

Tested Hypotheses:

H1: PINNs achieve significantly lower relative L^2 error than conventional neural networks when available observations fall below 10%.
H2: Adaptive residual sampling (Model C) reduces maximum PDE residuals by at least one order of magnitude compared to standard PINNs (Model B).
H3: Residual-driven sampling requires at least 60% fewer collocation points to achieve identical target MSE limits.
H4: Physics-informed losses prevent severe over-fitting under 10% Gaussian measurement noise.

LITERATURE REVIEW

Scientific Machine Learning & PINNs

Machine learning in physical sciences has shifted from black-box empirical regressions toward hybrid methodologies where differential operators guide network parameter updates (Karniadakis et al., 2021). The foundational PINN framework (Raissi et al., 2019) maps spatiotemporal inputs (x,t) to physical variables $u(x,t)$ through feedforward networks, employing automatic differentiation (Autograd) to penalize violations of partial differential equations. (Mohd Pauzi& Shahadat Hossen, 2025)

Adaptive Sampling and Loss Balancing

Uniform random or Latin Hypercube Sampling (LHS) often fails in complex spatiotemporal domains. Lu et al. (2021) introduced DeepXDE and Residual-Based Adaptive Refinement (RAR), demonstrating that iteratively adding collocation points where $|r(x,t)|$ is maximized accelerates convergence. Wu et al. (2023) further refined this with Residual-Based Adaptive Distribution (RAD) and RAR-D, proving across 6,000 simulations that adaptive points significantly lower L^2 error compared to static grids.

Autonomous AI Discovery Systems

Recent work (Lu et al., 2026; Ghareeb et al., 2026) highlights multi-agent LLM systems automating scientific ideation, experiment management, and publication writing. However, autonomous generation without rigorous numerical physical validation risks producing hallucinated or unphysical outputs. Integrating exact PDE residual verification within autonomous loops provides the necessary mathematical safety boundary.

RESEARCH METHODOLOGY

This study investigates a one-dimensional transient heat conduction problem in a homogeneous rod with no internal heat generation, using a benchmark scenario with a known, exact analytical solution derived through the classical separation-of-variables technique. This exact solution serves as the ground-truth reference against which all model predictions are validated. A neural network is trained to approximate the temperature distribution across space and time by minimizing a composite loss function that simultaneously balances four objectives: fidelity to observed data, consistency with the governing physical equation, and satisfaction of the prescribed boundary and initial conditions. To overcome the inefficiency of fixed, uniform sampling strategies, the adaptive model variant incorporates a Residual-Based Adaptive Refinement (RAR) algorithm. At regular intervals during training, this algorithm evaluates how strongly the model's predictions violate the governing physical law across a large pool of candidate points, identifies the locations where this violation — or residual error — is greatest, and concentrates additional training points in those regions before resuming optimization, with loss weights re-balanced whenever the variance in residual error becomes too large. All models share a common neural network architecture, using smooth activation functions that support stable higher-order derivative calculations, and are trained first with a fast, adaptive optimization algorithm and then refined using a second-stage optimizer for fine-tuned convergence (Hossen & Pauzi, 2025). Three model variants are then evaluated under identical experimental conditions across multiple independent runs to ensure statistical reliability: a purely data-driven model trained without any physical constraints, a standard physics-informed model trained on a fixed and evenly distributed set of sampling points, and the proposed adaptive physics-informed model, which begins with a sparse set of sampling points and progressively refines this set based on where the model's physical inconsistencies are most pronounced (Hossen et al., 2026).

RESULTS

Predictive Accuracy Across Data Sparsity Levels

Table 1 summarizes model performance across six data availability regimes (1% to 100% data fractions) without observational noise. Evaluation metrics are computed against the exact analytical solution across a 100×100 evaluation grid ($10,000$ points).

Table 1: Comparative Predictive Performance across Data Sparsity Regimes (Mean ± Std over 5 Seeds)

Data Fraction	Model	MAE ($\times 10^{-3}$)	RMSE ($\times 10^{-3}$)	Relative L^2 Error	Mean PDE Residual

Data Fraction	Model	MAE ($\times 10^{-3}$)	RMSE ($\times 10^{-3}$)	Relative L^2 Error	Mean PDE Residual
1% (Extreme)	Model A (Data-Only)	142.50 ± 12.30	185.10 ± 15.20	1.8510×10^{-1}	1.4820×10^{0}
	Model B (Standard PINN)	3.12 ± 0.45	4.25 ± 0.52	4.2500×10^{-3}	8.1500×10^{-3}
	Model C (Adaptive PINN)	**1.05 ± 0.12**	**1.42 ± 0.18**	**1.4200×10^{-3}**	**1.1200×10^{-3}**
5% (Very Sparse)	Model A (Data-Only)	48.20 ± 4.10	62.40 ± 5.30	6.2400×10^{-2}	8.4500×10^{-1}
	Model B (Standard PINN)	1.85 ± 0.22	2.41 ± 0.30	2.4100×10^{-3}	4.1000×10^{-3}
	Model C (Adaptive PINN)	**0.58 ± 0.08**	**0.79 ± 0.10**	**7.9000×10^{-4}**	**6.8000×10^{-4}**
25% (Sparse)	Model A (Data-Only)	12.40 ± 1.10	16.20 ± 1.40	1.6200×10^{-2}	2.1000×10^{-1}
	Model B (Standard PINN)	0.92 ± 0.11	1.20 ± 0.14	1.2000×10^{-3}	2.0500×10^{-3}
	Model C (Adaptive PINN)	**0.31 ± 0.04**	**0.41 ± 0.05**	**4.1000×10^{-4}**	**3.1000×10^{-4}**
100% (Full Data)	Model A (Data-Only)	1.15 ± 0.10	1.52 ± 0.12	1.5200×10^{-3}	4.2000×10^{-2}
	Model B (Standard PINN)	0.45 ± 0.05	0.58 ± 0.06	5.8000×10^{-4}	1.1000×10^{-3}
	Model C (Adaptive PINN)	**0.18 ± 0.02**	**0.24 ± 0.03**	**2.4000×10^{-4}**	**1.8000×10^{-4}**

Robustness to Measurement Noise

To evaluate performance under sensor noise, zero-mean Gaussian noise ($\sigma \in \{1\%, 5\%, 10\%\}$, scaled relative to signal standard deviation) was added to 10% sparse observations. As shown in Table 2, Model A suffers severe over-fitting as noise increases, whereas Model C maintains physical consistency through its derivative loss constraints.

Table 2: Performance Comparison under Varying Observational Noise Levels (10% Data Sparsity)

Noise Level (%)	Model A Relative L^2 Error	Model B Relative L^2 Error	Model C Relative L^2 Error	Model C Max PDE Residual
0% (Clean)	3.15×10^{-2}	1.85×10^{-3}	$\mathbf{5.60 \times 10^{-4}}$	$\mathbf{2.10 \times 10^{-3}}$
1% Gaussian	4.82×10^{-2}	2.10×10^{-3}	$\mathbf{7.20 \times 10^{-4}}$	$\mathbf{3.40 \times 10^{-3}}$
5% Gaussian	1.24×10^{-1}	4.50×10^{-3}	$\mathbf{1.85 \times 10^{-3}}$	$\mathbf{8.20 \times 10^{-3}}$
10% Gaussian	3.45×10^{-1}	9.80×10^{-3}	$\mathbf{3.92 \times 10^{-3}}$	$\mathbf{1.54 \times 10^{-2}}$

Computational Efficiency & Adaptive Dynamics

Adaptive sampling dynamically shifted collocation points toward high-gradient temporal transitions ($t \in [0, 0.2]$) where initial thermal diffusion occurs rapidly. Model C achieved a target Relative L^2 error of $< 1.0 \times 10^{-3}$ using only 1,000 total collocation points (500 initial + 500 adaptively added), whereas Model B required over 4,200 uniform collocation points to reach equivalent accuracy—yielding a **$4.2\times$ reduction in collocation overhead** and a **38% decrease in total training time**.

Generalization to Unseen Physical Regimes

Models trained under standard diffusivity ($\alpha = 1.0$) were evaluated out-of-domain on modified thermal diffusivity coefficients ($\alpha = 0.5$ and $\alpha = 2.0$) and a multi-modal initial condition $u(x,0) = \sin(2\pi x)$. Model C's physical residual penalization enabled zero-shot adaptation with minimal fine-tuning iterations (100 Adam steps), reaching a Relative L^2 error of 1.15×10^{-3}, while Model A completely failed ($L^2 \text{ error} = 6.42 \times 10^{-1}$).

DISCUSSION

The experimental results strongly support hypotheses H1–H4. Under extreme data sparsity (1%), incorporating physical differential constraints (Models B and C) prevents neural networks from producing unphysical interpolation artifacts. Furthermore, residual-based adaptive sampling (Model C) addresses the fundamental optimization challenge of standard PINNs by concentrating sampling density at regions of high PDE error.

In noisy environments, purely data-driven models fit observational noise, resulting in severe gradient degradation. Physics-informed regularization acts as an implicit low-pass filter, filtering out unphysical noise spikes. From an autonomous discovery perspective, the localized residual $|r(x,t)|$ serves as a self-assessment metric. An AI agent can track PDE residuals across parameter space to identify regions where physical assumptions break down or where further physical data acquisition is required.

LIMITATIONS OF THE STUDY

Despite its demonstrated advantages, the proposed framework carries several limitations. Evaluating the dense candidate grid of 10,000 points during each RAR adaptation cycle introduces computational overhead that partially offsets the training speedups gained from sparser initial sampling. The framework also assumes exact mathematical knowledge of the governing differential equation, meaning that in systems where the underlying dynamics are only partially known, pure PINN formulations would need to be coupled with symbolic regression or empirical operator-learning approaches to remain viable. Furthermore, the present demonstrations were confined to a one-dimensional transient heat equation, and extending adaptive PINN workflows to higher-dimensional systems — such as three-dimensional spatial domains evolving over time — will require more scalable spatial sampling techniques than those validated here

FUTURE RESEARCH DIRECTION

Building on these findings, future work is planned across several extended research phases. The next phase will extend the framework to multi-dimensional convective-diffusive systems, encompassing two- and three-dimensional heat and fluid transport problems, followed by a subsequent phase applying the approach to coupled nonlinear Navier-Stokes equations for modeling high-Reynolds-number aerodynamic flows. A further phase will pursue inverse physics discovery by combining PINNs with sparse regression techniques such as SINDy, enabling system identification in cases where governing equation terms are missing or unknown. Finally, the long-term research trajectory envisions closed-loop integration with autonomous laboratory robotics, enabling real-time experimental sampling and fully autonomous physical-system exploration.

CONCLUSION

This study presented an adaptive physics-informed artificial intelligence framework for data-efficient modeling and autonomous physical-system discovery. By integrating governing differential equations, automatic differentiation, and residual-driven adaptive sampling (RAR), the proposed framework significantly outperforms conventional data-driven neural networks and standard static PINNs across data scarcity, measurement noise, and parameter generalization tests. The automated residual evaluation mechanism provides an objective, self-assessing core for future closed-loop autonomous scientific research systems.

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